

Creating an Allotrope file format

ADFExport for OpenLab CDS ChemStation Edition



Figure 1. Word cloud: Allotrope Data Format.

Introduction

The diverse analytical techniques used in today's laboratories generate an array of proprietary data formats, which can be challenging to juggle. Wouldn't you rather have a common, universal, shareable and archive-ready format? The Allotrope Data Format, a standardized framework developed by the Allotrope Foundation, enables you to store data in a standardized way following the concept of semantic web and linked data. Additional benefits include increased data integrity, improved scientific reproducibility, and reduced manual effort especially in relation to paper-based work. This also improves the ability to find, share, and archive data. Finally, this enables data re-use in the context of the sample workflow starting at sample registration to data archiving across different software platforms.

The Allotrope Data Format is developed by the Allotrope Foundation, an international consortium of pharmaceutical, biopharmaceutical and other scientific research-intensive industries with the shared mission of a single, universal data format: *"Allotrope aims to make the intelligent analytical laboratory a reality – an automated laboratory where data, methods and hardware components are seamlessly shared among disparate platforms, and where one-click reports can be produced based on data generated by any analytical instrument with data integrity built-in by design."* - Allotrope Foundation. For detailed information please visit the website <https://www.allotrope.org>.

Saving data in the Allotrope Data Format

ADFExport for OpenLab CDS ChemStation revision 1.0 enables export of ChemStation data to ADF. It is available for stand alone or networked workstations of OpenLab CDS ChemStation Edition Revision C.01.09. The utility enables export of LC-UV ChemStation raw data acquired in single run mode. This can be done automatically after a single run via post-run macro. Alternatively one can export existing ChemStation data manually into ADF format by running the export tool via windows command line.

The Allotrope Data Format is based on HDF5. This is a platform independent file format which includes the following three parts: Data Description, Data Cube, and Data Package.

The **Data Description** is based on semantic web technology and linked data concepts using the W3C standardized RDF format (see <https://www.w3.org/RDF>). It stores analytical metadata as a data graph in a standardized and structured way. With the current basic export option, the data description contains metadata about LC-UV raw data stored in ADF data cube. As soon as the first LC-UV data model is released by the Allotrope Foundation much more contextual metadata can be written into the Data Description of ADF and more export options will be available.

The **Data Cube** contains analytical raw data which includes ChemStation LC-UV chromatograms and the corresponding UV spectra.

The **Data Package** is a universal data container filled with the original ChemStation files including all files and folders of the ChemStation .D folder.

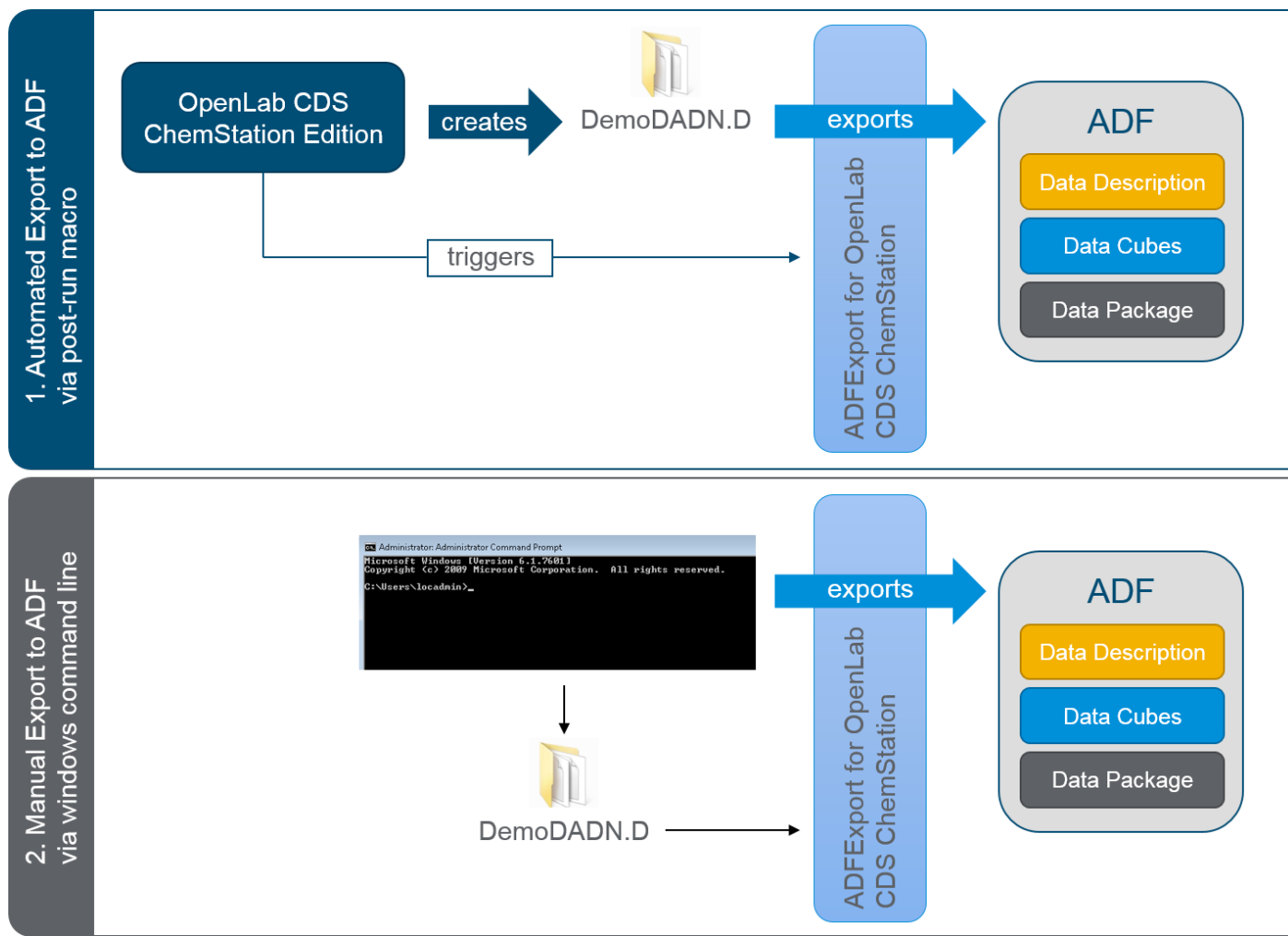


Figure 2. Supported workflows: 1. Automated export to ADF after a single run via post-run macro; 2. Manual export of existing ChemStation data via windows command line.

Reviewing data with the ADFExplorer

To browse the content of the created ADF file you can use the ADFExplorer released by the Allotrope Foundation (<https://www.allotrope.org>). Different views (tabular or graphical) are available to show the content of every part in more detail.

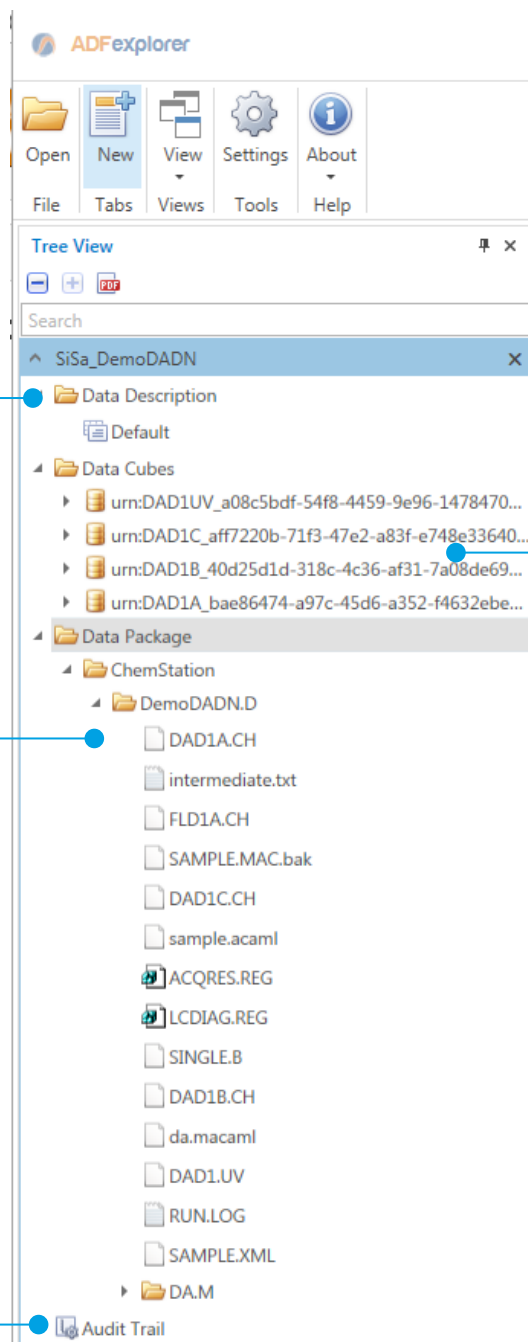
Data Description

Contains metadata about LC-UV raw data stored in ADF data cube.

Data Package

Contains original ChemStation files in a "ChemStation" subfolder.

ADF Audit trail



Data Cubes

Contains ChemStation LC-UV raw data (this demo data contain 3 chromatograms, signal DAD1A, DAD1B and DAD1C and one spectrum DAD1UV).

Figure 3. The content of ADF file SiSa_DemoDADN is displayed in the Tree View of ADFExplorer.

Conclusion

Driven by the pharmaceutical industry the Allotrope Foundation aims to develop a single common data format for any analytical technique. The goal is to facilitate the collection, exchange, and storage of data in the laboratory. ADFExport for OpenLab CDS ChemStation Edition provides an ADF export functionality for chromatography data. Currently LC-UV ChemStation raw data can be stored in the Allotrope Data Format. Plans are underway to support additional techniques and more contextual metadata in future software releases.

To learn more about OpenLab CDS ChemStation Edition visit, www.agilent.com/chem/openlab-cds-chemstation

To learn more about the Allotrope Foundation visit, <https://www.allotrope.org>

www.agilent.com/chem

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Printed in the USA, July 20, 2018
5994-0096EN

